

## **Correlation based approach to boundary conditions in concurrent multi-scale modeling**

<sup>1</sup>D. M. Nicholson,

<sup>1</sup>Oak Ridge National laboratory, P.O. Box 2008 MS-6164, Oak Ridge, TN, 27831, USA

As an example of closely coupled multiscale modeling we have explored the coupling of a region treated atomistically with molecular dynamics (MD) and a surrounding region treated as finite element (FE). Comparison will be made between conventional handshaking schemes and our proposed absorbing boundary conditions that are based on conservation of energy flux.

Further formal development of a correlation function based multiscale coupling based on an entropy functional of the pair correlation will be presented. The relationship between this correlation based approach and the atomic density functional and phase field crystal approaches will be discussed.

Acknowledgments: This research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory and by the Division of Materials Sciences and Engineering, Office of Basic Energy Science, U. S. Department of Energy managed by UT-Battelle LLC for the Department of Energy.

nicholsondm@ornl.gov